Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BM1
Title	:	RIBOSOMAL ELONGATION FACTOR G (EF-G) FUSIDIC ACID RESISTANT MUTANT G16V
Authors	:	Hansson, S.; Singh, R.; Gudkov, A.T.; Liljas, A.; Logan, D.T.
Deposited on	:	2005-03-09
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

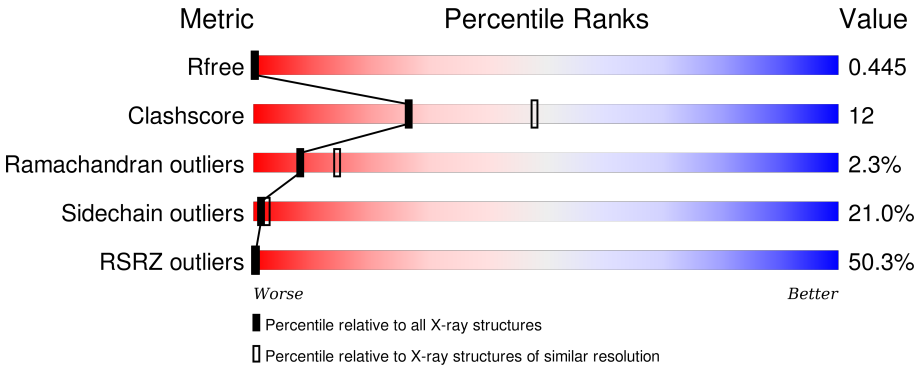
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	691	48% 57% 30% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5258 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

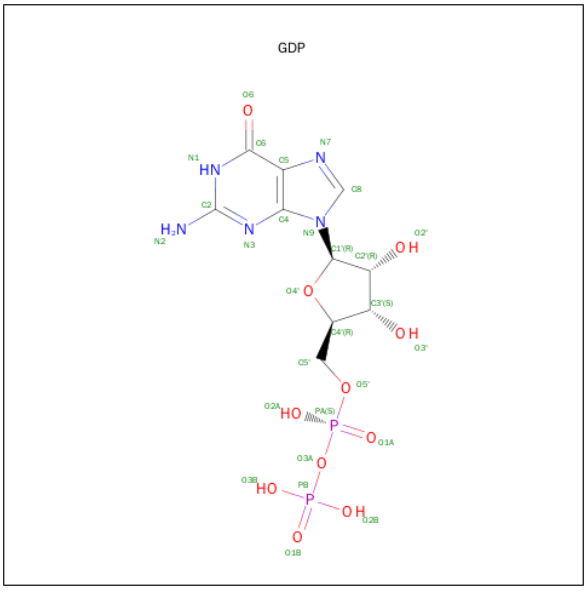
- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5167	3286	882	981	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	GLY	ENGINEERED MUTATION	UNP P13551

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

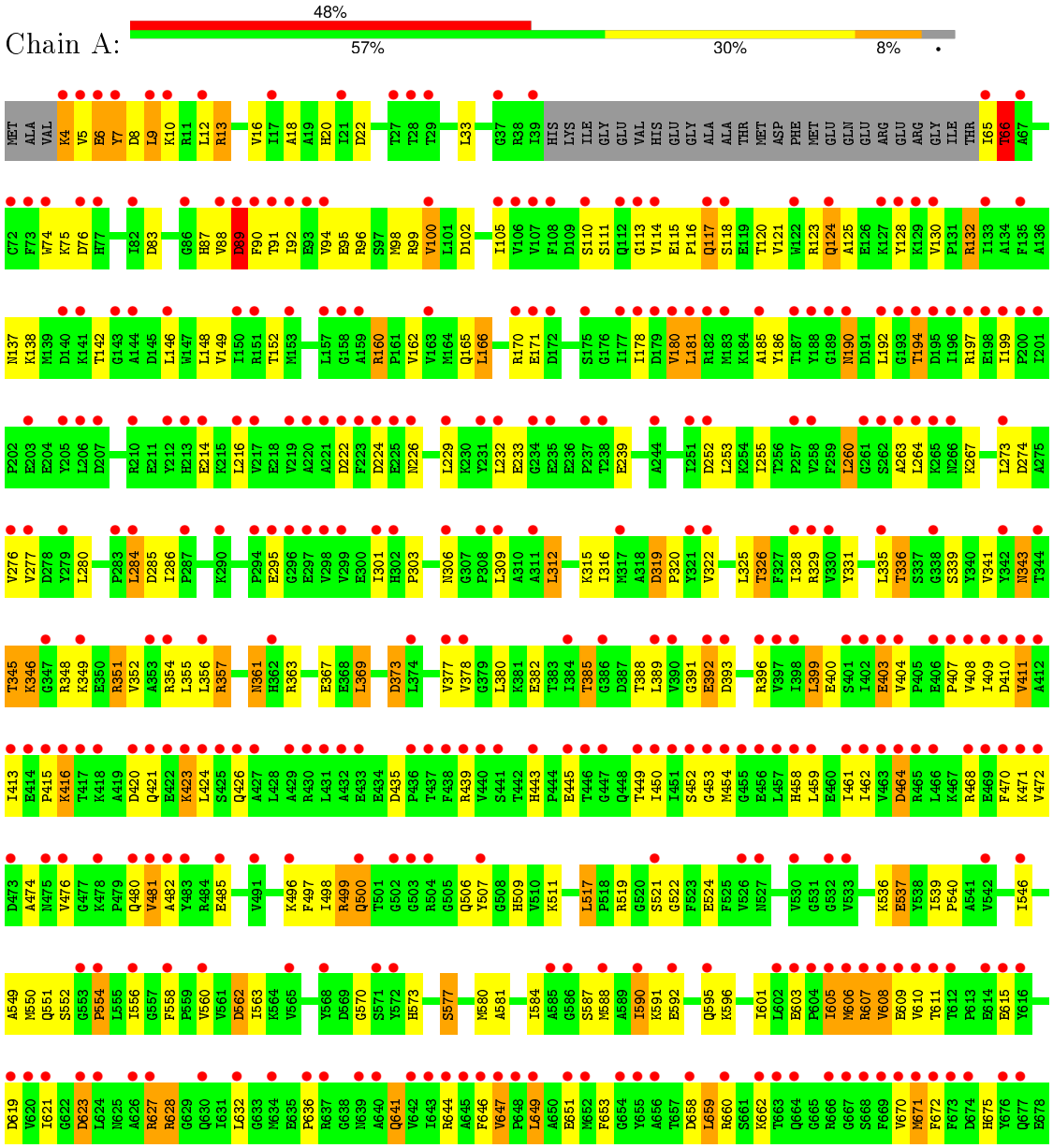
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0

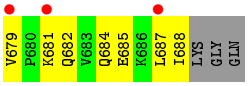
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ELONGATION FACTOR G

Chain A:




V679
P680
K681
Q682
V683
Q684
E685
K686
L687
I688
LYS
GLY
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.30Å 89.70Å 114.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.60 22.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.00-2.60) 98.7 (22.52-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.297 0.443 , 0.445	Depositor DCC
R_{free} test set	1247 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 24503 reflections	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.72	0/5264	0.93	23/7131 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	562	ASP	CB-CG-OD2	8.08	125.58	118.30
1	A	393	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	224	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	252	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	83	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	76	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	410	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	285	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	222	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	89	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	8	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	619	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	435	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	464	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	396	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	102	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	13	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	274	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	319	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	658	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	623	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	357	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5167	0	5230	127	9
2	A	28	0	12	1	0
3	A	1	0	0	0	1
4	A	62	0	0	10	0
All	All	5258	0	5242	127	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:HD22	1:A:192:LEU:H	1.23	0.82
1:A:190:ASN:ND2	1:A:192:LEU:H	1.76	0.81
1:A:636:PRO:HB3	1:A:641:GLN:HE21	1.45	0.81
1:A:361:ASN:HD22	1:A:361:ASN:H	1.27	0.81
1:A:632:LEU:HD21	1:A:646:PHE:CE2	2.18	0.79
1:A:165:GLN:NE2	1:A:260:LEU:H	1.82	0.77
1:A:132:ARG:CZ	4:A:2011:HOH:O	2.35	0.73
1:A:137:ASN:HD21	1:A:263:ALA:H	1.37	0.73
1:A:4:LYS:HA	1:A:5:VAL:C	2.15	0.67
1:A:580:MET:HG2	4:A:2055:HOH:O	1.95	0.66
1:A:90:PHE:O	1:A:670:VAL:HG12	1.95	0.65
1:A:165:GLN:HE21	1:A:260:LEU:H	1.44	0.64
1:A:18:ALA:HB1	1:A:121:VAL:HG21	1.79	0.62
1:A:415:PRO:HA	1:A:474:ALA:HB1	1.81	0.62
1:A:9:LEU:HD13	1:A:284:LEU:HD13	1.83	0.60
1:A:605:ILE:HG22	1:A:605:ILE:O	2.02	0.60
1:A:343:ASN:HD22	1:A:343:ASN:C	2.05	0.60
1:A:636:PRO:HB3	1:A:641:GLN:NE2	2.16	0.59
1:A:295:GLU:OE2	4:A:2034:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:O	1:A:117:GLN:HB2	2.04	0.58
1:A:316:ILE:CD1	1:A:326:THR:HB	2.35	0.57
1:A:610:VAL:HG13	1:A:659:LEU:HD11	1.85	0.57
1:A:550:MET:SD	1:A:563:ILE:HD11	2.45	0.57
1:A:546:ILE:HG23	1:A:590:ILE:HG13	1.87	0.57
1:A:113:GLY:HA2	1:A:149:VAL:HG22	1.87	0.56
1:A:391:GLY:O	1:A:392:GLU:CB	2.53	0.56
1:A:517:LEU:HD21	1:A:524:GLU:HG3	1.85	0.56
1:A:409:ILE:HD11	1:A:649:LEU:HD11	1.87	0.56
1:A:316:ILE:HG12	1:A:385:THR:HG22	1.87	0.55
1:A:89:ASP:O	1:A:124:GLN:NE2	2.40	0.55
1:A:326:THR:HG22	4:A:2039:HOH:O	2.05	0.55
1:A:485:GLU:O	1:A:560:VAL:HA	2.07	0.55
1:A:125:ALA:O	1:A:128:TYR:O	2.25	0.55
1:A:388:THR:HG23	1:A:399:LEU:HD22	1.87	0.54
1:A:415:PRO:HB2	1:A:420:ASP:HB3	1.90	0.54
1:A:160:ARG:HG2	1:A:255:ILE:HG22	1.90	0.54
1:A:536:LYS:O	1:A:537:GLU:CB	2.56	0.54
1:A:9:LEU:HD13	1:A:284:LEU:CD1	2.39	0.53
1:A:100:VAL:HG22	1:A:329:ARG:HB2	1.90	0.53
1:A:316:ILE:HD13	1:A:326:THR:HB	1.91	0.52
1:A:549:ALA:HB1	1:A:591:LYS:HD3	1.92	0.52
1:A:181:LEU:HD22	1:A:216:LEU:HD21	1.92	0.52
1:A:94:VAL:HG12	1:A:94:VAL:O	2.10	0.51
1:A:116:PRO:O	1:A:117:GLN:CB	2.59	0.51
1:A:409:ILE:CG1	1:A:649:LEU:HD11	2.42	0.50
1:A:603:GLU:CD	1:A:679:VAL:HG12	2.32	0.50
1:A:351:ARG:HB2	1:A:351:ARG:CZ	2.41	0.50
1:A:632:LEU:HD11	1:A:646:PHE:CE1	2.47	0.49
1:A:96:ARG:HG3	1:A:400:GLU:OE2	2.12	0.49
1:A:7:TYR:OH	1:A:9:LEU:HG	2.12	0.49
1:A:605:ILE:HG21	1:A:675:HIS:CE1	2.48	0.48
1:A:100:VAL:HG22	1:A:329:ARG:CB	2.43	0.48
1:A:549:ALA:HB3	1:A:590:ILE:CG2	2.43	0.48
1:A:351:ARG:HB2	1:A:351:ARG:NH2	2.29	0.48
1:A:148:LEU:O	1:A:152:THR:HG22	2.13	0.48
1:A:361:ASN:HD22	1:A:361:ASN:N	2.02	0.48
1:A:539:ILE:N	1:A:540:PRO:CD	2.76	0.48
1:A:536:LYS:O	1:A:537:GLU:CD	2.52	0.47
1:A:509:HIS:HD1	1:A:570:GLY:HA2	1.78	0.47
1:A:536:LYS:O	1:A:537:GLU:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:VAL:HG23	1:A:482:ALA:N	2.29	0.47
1:A:301:ILE:HD13	1:A:399:LEU:HD11	1.97	0.46
1:A:190:ASN:C	1:A:190:ASN:HD22	2.18	0.46
1:A:165:GLN:HA	1:A:178:ILE:O	2.14	0.46
1:A:319:ASP:OD1	1:A:363:ARG:NH2	2.44	0.46
1:A:506:GLN:HE21	1:A:581:ALA:HB2	1.80	0.46
1:A:65:ILE:O	1:A:66:THR:C	2.54	0.46
1:A:454:MET:CG	1:A:458:HIS:CD2	2.99	0.46
1:A:20:HIS:ND1	1:A:116:PRO:O	2.49	0.46
1:A:166:LEU:HD22	1:A:180:VAL:HG11	1.98	0.46
1:A:355:LEU:HD22	1:A:369:LEU:CD2	2.46	0.46
1:A:415:PRO:O	1:A:416:LYS:HB2	2.16	0.45
1:A:114:VAL:H	1:A:152:THR:HG21	1.81	0.45
1:A:325:LEU:HD21	1:A:356:LEU:HD12	1.98	0.45
1:A:458:HIS:ND1	1:A:462:ILE:HD11	2.32	0.45
1:A:5:VAL:O	1:A:6:GLU:C	2.55	0.45
1:A:345:THR:C	1:A:346:LYS:O	2.52	0.45
1:A:354:ARG:HB2	1:A:378:VAL:HB	1.98	0.45
1:A:411:VAL:O	1:A:450:ILE:HA	2.17	0.45
1:A:573:HIS:O	1:A:577:SER:HB2	2.17	0.45
1:A:536:LYS:O	1:A:537:GLU:CG	2.65	0.45
1:A:584:ILE:O	1:A:588:MET:HG3	2.17	0.44
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.47	0.44
1:A:361:ASN:H	1:A:361:ASN:ND2	2.06	0.44
1:A:609:GLU:HB3	1:A:670:VAL:CG2	2.47	0.44
1:A:409:ILE:O	1:A:452:SER:HA	2.18	0.44
1:A:497:PHE:CZ	1:A:499:ARG:HD2	2.53	0.44
1:A:607:ARG:C	4:A:2057:HOH:O	2.56	0.44
1:A:185:ALA:HB3	1:A:199:ILE:HG13	2.00	0.44
1:A:114:VAL:HG23	1:A:152:THR:HG23	2.01	0.43
1:A:336:THR:HG22	1:A:339:SER:HB3	1.99	0.43
1:A:312:LEU:O	1:A:328:ILE:HA	2.18	0.43
1:A:407:PRO:HA	1:A:453:GLY:O	2.19	0.43
1:A:186:TYR:HA	1:A:197:ARG:O	2.18	0.43
1:A:413:ILE:HG23	1:A:413:ILE:O	2.19	0.43
1:A:601:ILE:HG13	1:A:684:GLN:HE21	1.84	0.43
1:A:415:PRO:HG2	1:A:421:GLN:HG2	2.01	0.42
1:A:309:LEU:HD21	1:A:335:LEU:CD1	2.49	0.42
1:A:105:ILE:HD11	1:A:276:VAL:CG2	2.49	0.42
1:A:409:ILE:CG2	1:A:459:LEU:HD13	2.49	0.42
1:A:409:ILE:HG21	1:A:459:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ILE:HA	1:A:506:GLN:O	2.18	0.42
1:A:408:VAL:HG21	1:A:606:MET:HE2	2.01	0.42
1:A:423:LYS:HA	1:A:426:GLN:HB2	2.02	0.42
1:A:522:GLY:O	1:A:562:ASP:HA	2.19	0.42
1:A:115:GLU:O	1:A:118:SER:HB2	2.19	0.42
1:A:554:PRO:HB3	1:A:595:GLN:HG2	2.01	0.42
1:A:413:ILE:HD13	1:A:424:LEU:HD21	2.01	0.42
1:A:132:ARG:NH1	4:A:2011:HOH:O	2.49	0.41
1:A:671:MET:CG	4:A:2057:HOH:O	2.68	0.41
1:A:644:ARG:HB3	4:A:2058:HOH:O	2.20	0.41
1:A:409:ILE:CD1	1:A:649:LEU:HD11	2.50	0.41
1:A:138:LYS:HG2	2:A:1689:GDP:C6	2.55	0.41
1:A:608:VAL:CG2	1:A:647:VAL:CG1	2.99	0.41
1:A:627:ARG:HB2	1:A:651:GLU:O	2.21	0.41
1:A:357:ARG:NH1	1:A:373:ASP:OD2	2.54	0.41
1:A:74:TRP:CD1	1:A:75:LYS:HG2	2.56	0.41
1:A:123:ARG:HG3	1:A:611:THR:HG21	2.02	0.41
1:A:498:ILE:HG12	1:A:507:TYR:CD2	2.55	0.41
1:A:335:LEU:HD11	1:A:341:VAL:HG11	2.02	0.41
1:A:94:VAL:CG1	1:A:94:VAL:O	2.69	0.41
1:A:506:GLN:NE2	1:A:581:ALA:HB2	2.36	0.41
1:A:499:ARG:NE	4:A:2049:HOH:O	2.54	0.41
1:A:413:ILE:HD11	1:A:424:LEU:HD11	2.03	0.40
1:A:601:ILE:HG12	4:A:2048:HOH:O	2.22	0.40
1:A:303:PRO:HA	1:A:331:TYR:O	2.21	0.40
1:A:470:PHE:HB3	1:A:472:VAL:HG23	2.01	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:OE2	3:A:1690:MG:MG[3_555]	1.18	1.02
1:A:226:ASN:ND2	1:A:685:GLU:OE1[1_655]	1.49	0.71
1:A:367:GLU:OE1	1:A:500:GLN:OE1[1_655]	1.59	0.61
1:A:194:THR:O	1:A:521:SER:O[3_545]	2.05	0.15
1:A:367:GLU:CB	1:A:500:GLN:CB[1_655]	2.06	0.14
1:A:306:ASN:ND2	1:A:496:LYS:CE[1_655]	2.15	0.05
1:A:194:THR:CA	1:A:521:SER:O[3_545]	2.16	0.04
1:A:194:THR:OG1	1:A:521:SER:O[3_545]	2.17	0.03
1:A:367:GLU:CD	1:A:500:GLN:OE1[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	656/691 (95%)	578 (88%)	63 (10%)	15 (2%)	8 14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	416	LYS
1	A	537	GLU
1	A	91	THR
1	A	117	GLN
1	A	392	GLU
1	A	403	GLU
1	A	171	GLU
1	A	628	ARG
1	A	346	LYS
1	A	380	LEU
1	A	87	HIS
1	A	320	PRO
1	A	554	PRO
1	A	556	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	558/583 (96%)	441 (79%)	117 (21%)	1 2

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	GLU
1	A	7	TYR
1	A	9	LEU
1	A	10	LYS
1	A	12	LEU
1	A	13	ARG
1	A	16	VAL
1	A	22	ASP
1	A	33	LEU
1	A	66	THR
1	A	88	VAL
1	A	89	ASP
1	A	92	ILE
1	A	95	GLU
1	A	98	MET
1	A	99	ARG
1	A	100	VAL
1	A	110	SER
1	A	111	SER
1	A	120	THR
1	A	124	GLN
1	A	130	VAL
1	A	132	ARG
1	A	142	THR
1	A	146	LEU
1	A	160	ARG
1	A	162	VAL
1	A	166	LEU
1	A	170	ARG
1	A	180	VAL
1	A	181	LEU
1	A	190	ASN
1	A	194	THR
1	A	214	GLU
1	A	229	LEU
1	A	232	LEU
1	A	233	GLU
1	A	239	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	267	LYS
1	A	273	LEU
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	286	ILE
1	A	312	LEU
1	A	315	LYS
1	A	322	VAL
1	A	326	THR
1	A	336	THR
1	A	343	ASN
1	A	345	THR
1	A	348	ARG
1	A	349	LYS
1	A	351	ARG
1	A	352	VAL
1	A	361	ASN
1	A	369	LEU
1	A	373	ASP
1	A	377	VAL
1	A	382	GLU
1	A	385	THR
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	404	VAL
1	A	411	VAL
1	A	423	LYS
1	A	439	ARG
1	A	443	HIS
1	A	445	GLU
1	A	449	THR
1	A	461	ILE
1	A	464	ASP
1	A	468	ARG
1	A	471	LYS
1	A	476	VAL
1	A	480	GLN
1	A	481	VAL
1	A	499	ARG
1	A	500	GLN

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Mol	Chain	Res	Type
1	A	511	LYS
1	A	517	LEU
1	A	519	ARG
1	A	551	GLN
1	A	552	SER
1	A	558	PHE
1	A	577	SER
1	A	587	SER
1	A	590	ILE
1	A	592	GLU
1	A	596	LYS
1	A	605	ILE
1	A	606	MET
1	A	607	ARG
1	A	608	VAL
1	A	615	GLU
1	A	621	ILE
1	A	623	ASP
1	A	627	ARG
1	A	628	ARG
1	A	641	GLN
1	A	647	VAL
1	A	649	LEU
1	A	653	PHE
1	A	659	LEU
1	A	660	ARG
1	A	662	LYS
1	A	671	MET
1	A	672	PHE
1	A	681	LYS
1	A	682	GLN
1	A	687	LEU
1	A	688	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	124	GLN
1	A	137	ASN
1	A	154	GLN
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	208	GLN
1	A	343	ASN
1	A	361	ASN
1	A	448	GLN
1	A	480	GLN
1	A	506	GLN
1	A	551	GLN
1	A	630	GLN
1	A	641	GLN
1	A	675	HIS
1	A	677	GLN
1	A	684	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	A	1689	3	23,30,30	1.31	3 (13%)	30,47,47	1.96	8 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	1689	3	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1689	GDP	O4'-C1'	-3.27	1.37	1.41
2	A	1689	GDP	C2-N1	2.01	1.39	1.35
2	A	1689	GDP	C6-N1	3.27	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1689	GDP	N3-C2-N1	-4.88	120.02	127.44
2	A	1689	GDP	C5-C6-N1	-4.30	117.71	123.59
2	A	1689	GDP	C1'-N9-C4	-2.99	122.42	126.94
2	A	1689	GDP	O3A-PA-O5'	-2.93	95.17	102.94
2	A	1689	GDP	PA-O3A-PB	-2.63	123.83	132.67
2	A	1689	GDP	O4'-C1'-N9	2.42	113.17	108.10
2	A	1689	GDP	O3B-PB-O2B	2.83	118.15	107.38
2	A	1689	GDP	C6-N1-C2	4.08	121.60	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1689	GDP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	660/691 (95%)	2.35	332 (50%)	0	0	29, 50, 115, 126	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	ALA	13.1
1	A	284	LEU	12.6
1	A	640	ALA	9.3
1	A	263	ALA	9.2
1	A	626	ALA	8.9
1	A	232	LEU	8.9
1	A	645	ALA	8.3
1	A	470	PHE	8.2
1	A	402	ILE	7.2
1	A	471	LYS	7.0
1	A	296	GLY	6.5
1	A	201	ILE	6.4
1	A	670	VAL	6.3
1	A	656	ALA	6.1
1	A	669	PHE	6.1
1	A	473	ASP	6.1
1	A	663	THR	6.1
1	A	446	THR	6.0
1	A	668	SER	6.0
1	A	9	LEU	5.9
1	A	431	LEU	5.9
1	A	413	ILE	5.9
1	A	171	GLU	5.6
1	A	465	ARG	5.6
1	A	384	ILE	5.6
1	A	447	GLY	5.3
1	A	301	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	426	GLN	5.3
1	A	6	GLU	5.2
1	A	619	ASP	5.2
1	A	94	VAL	5.2
1	A	667	GLY	5.2
1	A	455	GLY	5.1
1	A	415	PRO	5.1
1	A	637	ARG	5.0
1	A	445	GLU	5.0
1	A	404	VAL	5.0
1	A	91	THR	4.9
1	A	408	VAL	4.9
1	A	113	GLY	4.9
1	A	462	ILE	4.8
1	A	440	VAL	4.7
1	A	283	PRO	4.7
1	A	226	ASN	4.7
1	A	86	GLY	4.7
1	A	114	VAL	4.6
1	A	655	TYR	4.6
1	A	308	PRO	4.6
1	A	344	THR	4.5
1	A	608	VAL	4.5
1	A	5	VAL	4.5
1	A	128	TYR	4.5
1	A	235	GLU	4.5
1	A	129	LYS	4.4
1	A	237	PRO	4.4
1	A	611	THR	4.4
1	A	652	MET	4.3
1	A	674	ASP	4.3
1	A	441	SER	4.3
1	A	632	LEU	4.3
1	A	92	ILE	4.2
1	A	302	HIS	4.2
1	A	194	THR	4.2
1	A	88	VAL	4.2
1	A	647	VAL	4.2
1	A	604	PRO	4.2
1	A	609	GLU	4.2
1	A	430	ARG	4.2
1	A	73	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	482	ALA	4.2
1	A	472	VAL	4.1
1	A	177	ILE	4.1
1	A	610	VAL	4.1
1	A	586	GLY	4.0
1	A	612	THR	4.0
1	A	185	ALA	4.0
1	A	418	LYS	4.0
1	A	620	VAL	4.0
1	A	77	HIS	4.0
1	A	110	SER	4.0
1	A	244	ALA	3.9
1	A	295	GLU	3.9
1	A	90	PHE	3.9
1	A	349	LYS	3.9
1	A	133	ILE	3.9
1	A	627	ARG	3.9
1	A	93	GLU	3.9
1	A	37	GLY	3.9
1	A	181	LEU	3.8
1	A	225	GLU	3.8
1	A	362	HIS	3.8
1	A	39	ILE	3.8
1	A	106	VAL	3.8
1	A	646	PHE	3.8
1	A	251	ILE	3.8
1	A	159	ALA	3.8
1	A	213	HIS	3.7
1	A	217	VAL	3.7
1	A	258	VAL	3.7
1	A	648	PRO	3.7
1	A	432	ALA	3.7
1	A	195	ASP	3.7
1	A	322	VAL	3.7
1	A	453	GLY	3.7
1	A	273	LEU	3.7
1	A	82	ILE	3.7
1	A	660	ARG	3.7
1	A	298	VAL	3.6
1	A	89	ASP	3.6
1	A	203	GLU	3.6
1	A	463	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	416	LYS	3.6
1	A	644	ARG	3.6
1	A	666	ARG	3.6
1	A	216	LEU	3.6
1	A	189	GLY	3.6
1	A	393	ASP	3.6
1	A	238	THR	3.5
1	A	478	LYS	3.5
1	A	397	VAL	3.5
1	A	532	GLY	3.5
1	A	135	PHE	3.4
1	A	424	LEU	3.4
1	A	4	LYS	3.4
1	A	234	GLY	3.4
1	A	502	GLY	3.4
1	A	469	GLU	3.4
1	A	616	TYR	3.4
1	A	452	SER	3.4
1	A	124	GLN	3.4
1	A	214	GLU	3.4
1	A	542	VAL	3.4
1	A	672	PHE	3.4
1	A	671	MET	3.4
1	A	461	ILE	3.4
1	A	639	ASN	3.4
1	A	206	LEU	3.3
1	A	374	LEU	3.3
1	A	407	PRO	3.3
1	A	422	GLU	3.3
1	A	158	GLY	3.3
1	A	205	TYR	3.3
1	A	317	MET	3.3
1	A	433	GLU	3.3
1	A	572	TYR	3.3
1	A	229	LEU	3.2
1	A	636	PRO	3.2
1	A	279	TYR	3.2
1	A	676	TYR	3.2
1	A	21	ILE	3.2
1	A	439	ARG	3.2
1	A	112	GLN	3.2
1	A	414	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	3.1
1	A	649	LEU	3.1
1	A	588	MET	3.1
1	A	560	VAL	3.1
1	A	183	MET	3.1
1	A	454	MET	3.1
1	A	290	LYS	3.1
1	A	679	VAL	3.1
1	A	417	THR	3.1
1	A	193	GLY	3.1
1	A	451	ILE	3.0
1	A	480	GLN	3.0
1	A	585	ALA	3.0
1	A	687	LEU	3.0
1	A	118	SER	3.0
1	A	438	PHE	3.0
1	A	328	ILE	3.0
1	A	403	GLU	3.0
1	A	127	LYS	3.0
1	A	7	TYR	3.0
1	A	223	PHE	3.0
1	A	571	SER	3.0
1	A	153	MET	3.0
1	A	623	ASP	3.0
1	A	107	VAL	3.0
1	A	421	GLN	3.0
1	A	681	LYS	2.9
1	A	252	ASP	2.9
1	A	556	ILE	2.9
1	A	10	LYS	2.9
1	A	178	ILE	2.9
1	A	457	LEU	2.9
1	A	664	GLN	2.9
1	A	182	ARG	2.9
1	A	262	SER	2.9
1	A	496	LYS	2.9
1	A	500	GLN	2.9
1	A	299	VAL	2.9
1	A	67	ALA	2.9
1	A	231	TYR	2.9
1	A	427	ALA	2.9
1	A	475	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	481	VAL	2.8
1	A	654	GLY	2.8
1	A	188	TYR	2.8
1	A	459	LEU	2.8
1	A	146	LEU	2.8
1	A	409	ILE	2.8
1	A	553	GLY	2.8
1	A	144	ALA	2.8
1	A	187	THR	2.8
1	A	199	ILE	2.8
1	A	621	ILE	2.8
1	A	330	VAL	2.8
1	A	554	PRO	2.8
1	A	306	ASN	2.8
1	A	483	TYR	2.7
1	A	643	ILE	2.7
1	A	207	ASP	2.7
1	A	347	GLY	2.7
1	A	130	VAL	2.7
1	A	163	VAL	2.7
1	A	277	VAL	2.7
1	A	630	GLN	2.7
1	A	76	ASP	2.7
1	A	212	TYR	2.7
1	A	219	VAL	2.7
1	A	658	ASP	2.7
1	A	311	ALA	2.7
1	A	392	GLU	2.7
1	A	12	LEU	2.7
1	A	466	LEU	2.7
1	A	29	THR	2.7
1	A	192	LEU	2.6
1	A	504	ARG	2.6
1	A	190	ASN	2.6
1	A	200	PRO	2.6
1	A	425	SER	2.6
1	A	108	PHE	2.6
1	A	401	SER	2.6
1	A	606	MET	2.6
1	A	338	GLY	2.6
1	A	150	ILE	2.6
1	A	533	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	420	ASP	2.6
1	A	329	ARG	2.6
1	A	450	ILE	2.6
1	A	449	THR	2.6
1	A	170	ARG	2.6
1	A	634	MET	2.6
1	A	398	ILE	2.6
1	A	503	GLY	2.5
1	A	321	TYR	2.5
1	A	276	VAL	2.5
1	A	412	ALA	2.5
1	A	179	ASP	2.5
1	A	468	ARG	2.5
1	A	507	TYR	2.5
1	A	456	GLU	2.5
1	A	485	GLU	2.5
1	A	406	GLU	2.5
1	A	437	THR	2.5
1	A	342	TYR	2.5
1	A	546	ILE	2.4
1	A	464	ASP	2.4
1	A	266	ASN	2.4
1	A	264	LEU	2.4
1	A	607	ARG	2.4
1	A	105	ILE	2.4
1	A	377	VAL	2.4
1	A	222	ASP	2.4
1	A	294	PRO	2.4
1	A	335	LEU	2.4
1	A	386	GLY	2.4
1	A	521	SER	2.4
1	A	180	VAL	2.4
1	A	353	ALA	2.4
1	A	74	TRP	2.4
1	A	257	PRO	2.3
1	A	122	TRP	2.3
1	A	423	LYS	2.3
1	A	614	GLU	2.3
1	A	605	ILE	2.3
1	A	224	ASP	2.3
1	A	100	VAL	2.3
1	A	642	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	651	GLU	2.3
1	A	287	PRO	2.3
1	A	615	GLU	2.3
1	A	389	LEU	2.3
1	A	378	VAL	2.3
1	A	595	GLN	2.3
1	A	390	VAL	2.2
1	A	28	THR	2.2
1	A	568	TYR	2.2
1	A	673	PHE	2.2
1	A	297	GLU	2.2
1	A	141	LYS	2.2
1	A	590	ILE	2.2
1	A	265	LYS	2.2
1	A	143	GLY	2.2
1	A	220	ALA	2.2
1	A	526	VAL	2.2
1	A	565	VAL	2.2
1	A	65	ILE	2.2
1	A	117	GLN	2.2
1	A	677	GLN	2.2
1	A	261	GLY	2.2
1	A	436	PRO	2.2
1	A	210	ARG	2.2
1	A	411	VAL	2.2
1	A	175	SER	2.1
1	A	396	ARG	2.1
1	A	443	HIS	2.1
1	A	476	VAL	2.1
1	A	602	LEU	2.1
1	A	196	ILE	2.1
1	A	27	THR	2.1
1	A	309	LEU	2.1
1	A	172	ASP	2.1
1	A	221	ALA	2.1
1	A	354	ARG	2.1
1	A	157	LEU	2.1
1	A	356	LEU	2.1
1	A	592	GLU	2.1
1	A	491	VAL	2.1
1	A	17	ILE	2.1
1	A	458	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLU	2.1
1	A	603	GLU	2.1
1	A	624	LEU	2.1
1	A	662	LYS	2.1
1	A	527	ASN	2.0
1	A	410	ASP	2.0
1	A	72	CYS	2.0
1	A	530	VAL	2.0
1	A	197	ARG	2.0
1	A	151	ARG	2.0
1	A	558	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GDP	A	1689	28/28	0.74	0.29	-0.52	25,36,40,41	0
3	MG	A	1690	1/1	0.91	0.17	-	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.